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THE USE OF SEDIMENT-TRACE ELEMENT GEOCHEMICAL MODELS FOR THE IDENTIFICATION OF LOCAL FLUVIAL BASELINE CONCENTRATIONS

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ABSTRACT Studies have demonstrated the utility of fluvial bed sediment chemical data in assessing local water-quality conditions. However, establishing local background trace element levels can be difficult. Reference to published average concentrations or the use of dated cores are often of little use in small areas of diverse local petrology, geology, land use, or hydrology. An alternative approach entails the construction of a series of sediment-trace element predictive models based on data from environmentally diverse but unaffected areas. Predicted values could provide a measure of local background concentrations and comparison with actual measured concentrations could identify elevated trace elements and affected sites. Such a model set was developed from surface bed sediments collected nationwide in the United States. Tests of the models in a small Louisiana basin indicated that they could be used to establish local trace element background levels, but required recalibration to account for local geochemical conditions outside the range of samples used to generate the nationwide models.

INTRODUCTION

The basic goal of most chemically oriented water-quality studies is to describe or evaluate existing conditions and to determine whether the study area has been naturally or anthropogenically affected. Historically, water-quality studies have focused on the collection and subsequent analysis of water samples (Feltz, 1980; Forstner & Wittmann, 1981; Horowitz, 1985). In most aquatic systems, however, the concentrations of trace elements associated with sediments are far greater than the concentrations dissolved in the water column (Forstner & Wittmann, 1981; Salomons & Forstner, 1984, Horowitz, 1985; Meybeck & Helmer, 1989). The strong association of numerous trace elements with sediments means that the distribution, transport, and availability of these constituents cannot be evaluated solely by the sampling and analysis of the dissolved phase (e.g., Ongley, et al., 1988). Further, there is ample evidence that fluvial-bed sediment sampling and subsequent chemical analysis can provide an accurate indication of local water-quality conditions, without many of the difficulties associated with similar attempts involving water sampling and analysis (Feltz, 1980; Forstner & Wittmann, 1981; Ongley, et al., 1988; Meybeck & Helmer, 1989).

When sediment-trace element concentrations are markedly elevated, simple reconnaissance surveys usually suffice to delineate the spatial distributions of the elements of concern. However, in areas of relatively low-level chemical inputs, affected areas are more difficult to identify. In such cases, local background trace element concentrations have to be established to identify elevated trace elements and their spatial or temporal distributions (e.g., Forstner & Wittmann, 1981; Salomons & Forstner, 1984). Several means have been employed to establish local background concentrations; these include: 1) the average composition of some local rock type(s), 2) dated sediment cores which provide a historical chemical record for the specific site under investigation and 3) chemical averages for recent sediments from relatively unaffected areas having similar local geologies (Turekian & Wedepohl, 1961; Wedepohl, 1969; Thomas, 1972; Aston, et al., 1973; Forstner & Wittmann, 1981; Salomons & Forstner, 1984). All three methods can have major drawbacks for establishing local trace element background levels, especially in fluvial systems (Forstner & Wittmann, 1981; Salomons & Forstner, 1984; Horowitz, 1985).

Reference to, and comparison with various published average rock compositions are often of little use in fluvial systems due to diverse geology, petrology, land-use or hydrology. Therefore, a thorough knowledge of the local geology and petrology is required prior to estimating the influence of different rock types on the composition of local sediments (Forstner & Wittmann, 1981). Even then, the published chemical averages for different rock types commonly lack trace element data entirely, or cover concentration ranges that are either too broad or too narrow, to permit accurate estimates of local background concentrations.

Unlike lakes, rivers usually lack sufficiently thick sediment deposits to allow coring and subsequent chemical analysis that could permit an evaluation of long-term temporal trends and the identification of local trace element background levels. Even when thick sediment deposits are available, the geochemical record is often inappropriate for establishing temporal trends or background levels due to post-depositional physical, chemical, or biological disturbances which tend to 'smear' the geochemical record (e.g., Forstner & Wittmann, 1981; Horowitz, 1985).

An alternative approach to the above-cited procedures is to collect and analyze a large number of sediment samples from relatively unaffected areas and using these data, develop a set of average background concentrations. Such averages should be developed for basins that have similar geologic, petrologic, and hydrologic conditions to the basin under study. Further, such averages would have to account for the affects of the various physical and chemical parameters (geochemical factors) such as grain size, surface area, and the concentration of various geochemical substrates which affect the capacity of sediments to concentrate and retain trace elements, before an adequate comparison could be made (Jones & Bowser, 1978; Forstner & Wittmann, 1981; Salomons & Forstner, 1984; Horowitz, 1985; Horowitz & Elrick, 1987).

Due to all the potential problems associated with defining useful average concentrations, it might prove more efficacious to develop a set of sediment-trace element predictive models that incorporate some or all of the geochemical factors, known to affect sediment-trace element concentrations. The models generated by using these geochemical factors as independent variables might then be used to establish local trace element background concentrations. Provided the models were based on a diverse suite of unimpacted sediment samples, they could be viewed as operational definitions of normal background levels. The advantage of this type of approach is that the models permit the comparison of trace element concentrations between locally derived samples and national or global averages derived from samples having substantially different geochemical factors. These comparisons can be made because the trace element data have been 'normalized' for those factors which typically make intercomparisons from dissimilar areas difficult or impossible. Thus, the collection and subsequent physical and chemical analysis of a set of sediment samples from a local basin, followed by a comparison of the predicted concentrations from the models (developed from data from unaffected areas) with the measured concentrations from the local samples, could be used to identify suspected elevated trace elements or affected sites.

The purpose of this paper is to describe the development of a set of sediment-trace element predictive models which operationally define trace element background levels which could be used to identify naturally or anthropogenically affected sites. Further, the paper describes the initial use and testing of these models in a small basin in Louisiana.

SAMPLE COLLECTION, TREATMENT, AND ANALYTICAL METHODS

A total of 61 bulk surface oxidized bed sediment samples were collected in and around the United States from sites assumed to be unaffected by anthropogenic influences to provide data for the development of the predictive models. Care was taken to ensure that the sampling devices did not contaminate the sediment samples and that sample integrity was maintained (e.g., loss of fines was limited through the use of appropriate sampling devices and techniques).

Prior to analysis, the samples were freeze-dried (Horowitz & Elrick, 1987; Horowitz & Elrick, 1988). Chemical analyses for Fe, Mn, Al, Ti, Cu, Zn, Cd, Pb, Ni, Co, Cr, As, Sb, Se, and Hg were performed using an HNO_3-HF-$HClO_4$ digestion and AAS quantitation (Horowitz & Elrick, 1987; Horowitz, et al., 1989). Total organic carbon (TOC) was determined, on sample aliquots pretreated with 10% HCl using an IR carbon analyzer. Loss on ignition (LOI) was used as a measure of the total organic matter in the samples. Other organic matter (OOM) was determined by subtracting TOC from LOI. Operationally defined geochemical substrates [Mn oxides (Mn· MnO_2), reactive Fe (Fe·MnO_2), amorphous Fe oxides (Fe·Fe_2O_3) and total extractable Fe (ΣEx·Fe) and Mn (ΣEx·Mn)] were determined sequentially on dried, unground aliquots by using a selection of commonly employed analytical techniques (Horowitz & Elrick, 1989)). Grain-size distributions/separations were made following the procedures of Horowitz & Elrick (1986), which consisted of sieving and air elutriation. Mean grain sizes (Mz) were calculated for each sample from percentiles determined on cumulative curves. Surface area (SA) was determined on appropriately sized sample aliquots using a single point BET method following the procedures of Horowitz & Elrick (1987).

MODEL DEVELOPMENT

Statistical Procedures

For most of the parameters, it was apparent that the samples displayed a wide range in values. The chemical concentrations were within the ranges reported for standard shales, thus supporting the contention that the samples were collected from non-anthropogenically affected sites (Turekian & Wedepohl, 1961)). A comparison of the mean and median values indicated that all the chemical and physical data were positively skewed. Therefore, prior to calculating the models, all data were log-transformed.

Attempts to develop models for the entire data set were not completely successful. Although models could be calculated for all the trace elements of interest, there were several difficulties. Scatterplots of trace elements and the various geochemical factors indicated that the data separated into two groups, dependent on Mz. The crossover point for these factors seemed to occur between an Mz of 63 and 125µm. The fact that correlation coefficients calculated for the trace element concentrations and the determined geochemical factors for the >125-µm and the <125-µm sample data sets were similar to those coefficients calculated for the entire data set confirmed that the crossover point occurred between 63 and 125µm.

TABLE 1 Summary of Single-Element, Nationwide, Multiple Linear Regression Models.

<125 µm Models Element	Components	n^*	$R^@$	$R'^{2\#}$	$\bar{x}^+$
Cu	Al, LOI, Fe·Fe_2O_3	21	.93	.84	20.
Zn	Al, Fe·MnO_2, LOI	21	.94	.87	88.
Pb	SA, OOM, Ti	19	.86	.70	23.
Cr	OOM, Fe, SA	21	.91	.80	51.
Ni	Al, TOC	18	.96	.91	25.
Co	Ti, %<2µm	19	.89	.77	17.
As	Fe, %<125µn	19	.88	.74	7.0
Sb	Al, %<63µm, Mn·MnO_2	19	.88	.73	0.6
Se	OOM, SA, Ti	21	.88	.74	0.4
Hg	Fe·Fe_2O_3, Mn·MnO_2	21	.89	.76	0.05
>125 µm Models					
Cu	LOI, Al, Ti	38	.93	.85	10.
Zn	Fe·Fe_2O_3, Al	40	.94	.87	48.
Pb	Al, Ti, Mn, %<125µm	33	.88	.74	20.
Cr	Fe·Fe_2O_3, Ti, Al	40	.89	.77	28.
Ni	Fe·Fe_2O_3, Al	39	.86	.71	16.
Co	Fe, ΣEx·Mn	34	.91	.81	14.
As	SA, Fe	39	.87	.75	7.0
Sb	SA, Fe, Mz	34	.86	.71	0.5
Se	LOI, Al	20	.85	.70	0.3
Hg	Fe_2O_3, Al	29	.87	.74	0.06

[*] number of samples modelled

[@] correlation coefficients for the relation between the predicted and the measured concentrations

[#] adjusted square of the correlation coefficients for the predicted and the measured concentrations

[+] mean concentration of the elements in mg kg^{-1}

A series of models were then calculated for each trace element using the two separate sample data sets. One sample having an Mz of 125µm could fit into either group. The model results (the <125µm and the >125µm models incorporated different independent variables) and the behavior of this sample, seem to be consistent with the view that the factors affecting sediment-associated trace element chemistry are grain-size dependent, and the influence of various geochemical factors shift in importance around 125µm. Once a model was generated, the independent variables were examined for collinearity. Wherever possible, attempts were made to reduce correlations to less than 0.5, between independent variables, either by substitution or elimination. A residual analysis then was performed to determine if any of the individual data points represented outliers that exerted a high influence on the final model. In some instances, the residual analyses led to the removal of a limited number of samples from the data set where there was a 'lack of fit' (i.e., the residual analysis indicated a non-random relation between a dependent and an independent variable). Where this occurred, the problematic data points were removed, and a new model was calculated using the smaller data set.

Multiple linear regression models

The results for the <125-µm and the >125-µm models are presented in Table 1. The R'^2 (adjusted R^2) for the <125-µm models ranged from a low of 0.70 (Pb) to a high of 0.91 (Ni); for the >125-µm models, the range was 0.70 (Se) to 0.87 (Zn). Many of the independent variables found in the models were expected, based upon prior work (Forstner & Wittmann, 1981; Salomons & Forstner, 1984; Horowitz, 1985). On the other hand, several factors were included in some of the models that were not expected. In some instances, the appearance of these 'atypical' factors resulted from the eliminations/substitutions required to reduce collinearity. It should be understood that the independent variables used in the models were evaluated and selected on the basis of statistical considerations (e.g., to eliminate collinearity) and on predictive capability (e.g., how closely the models could predict trace element concentrations based on R, and on how well the models could account for measured trace element concentration variances based on R'^2), and many may not reflect cause-and-effect relations.

Correlation coefficients were calculated for predicted and actual concentrations to provide an indication of how closely the models estimated the actual trace element concentrations (R in Table 1). The correlation coefficients ranged from a low of 0.85 (Se) to a high of 0.96 (Ni). Considering the diversity of the environments from which the samples were collected (lakes, large rivers, small rivers, etc.) and the fairly wide range of analytical concentrations for the two data sets, the models explain a high percentage of the observed trace element variations.

Principal component and cross-product analyses

A principal component analysis (PCA) was performed on all the independent variables used to construct both the <125-µm and the >125-µm single-element models to determine if the variables could be separated into groups of environmentally rational factors (factors that are in accord with the known geochemical behavior of the various trace elements). Three principal components were retained for the <125-µm models. On the basis of the correlations between the original variables and the components, the three principal components retained were interpreted as representing background contributions (Fe, Al, and Ti), organic matter (LOI and OOM), and coatings (Fe·MnO_2, Fe· Fe_2O_3, and ΣEx·Fe). Two principal components were retained for the >125-µm models. On the basis of correlations between the original variables and the components, the two principal components retained were interpreted as representing background (Fe, Al, and Ti) and coatings (TOC, LOI, surface area, Fe·MnO_2, Fe·Fe_2O_3, and ΣEx·Mn).

Two additional sets of models were developed by using the retained principal component scores (PCA) and the principal component scores and component cross-products (PCA/XP) as independent variables; surface area for the <125-µm models and Mz for the >125-µm models also were included as potential independent variables owing to their incorporation in the single-element models. On the basis of the R'^2, for the great majority of elements, the new models either offered no substantial improvement, or were markedly poorer than the single-element models in explaining the observed trace element variance.

Comparisons of the calculated results (predicted concentrations compared to actual concentrations and the absolute means of the residuals compared to the analytical errors), from the single-element, PCA, and PCA/XP models indicated that the single-element models were the most successful (in terms of the R'^2) for the great majority of trace elements. Thus, for most of the elements investigated, the PCA or PCA/XP models would require a great deal more analytical work (the determination of 10 to 13 geochemical factors) than many of the single-element models, for little or no improvement in predictive capability.

MODEL UTILIZATION

Sample outliers

Eight of the twenty models [Pb (<125-µm, >125-µm), As (<125-µm, >125-µm), Sb (<125-µm, >125-µm), Co (<125-µm), Hg (>125-µm)] were calculated after the removal of data outliers. These (data) samples were removed from the models either as a result of the residual analyses or because initial calculations indicated that they caused major reductions in the R'^2 values. In most of the latter cases, environmental rationales could be found to justify their removal. Those models which encompassed the entire data set could serve effectively as screening tools; if a new sample did not fit these models, it might indicate the need to further investigate that sampling site, because it could be naturally or anthropogenically affected. The exclusion of a new sample from those models that did not encompass the entire data set also could indicate that the sampling site might be naturally or anthropogenically affected. However, this conclusion is less certain than for the models that encompassed all the samples because there seem to be some limits to the applicability of these models in certain environmental settings or for certain chemical ranges (removal of model outliers). In this context, it should be noted that many of the sample outliers do not contain the highest concentrations of the various trace elements in the group; thus, concentration, *per se*, or comparison of sample concentrations with broad published averages such as for typical shales (e.g., Turekian & Wedepohl, 1961), would not have been sufficient to identify this type of sample.

Model-generated trace element background levels

The models might provide a potential definition of an 'average' or background sediment-associated trace element concentration. Since the models were developed from data obtained from unaffected sediments, samples collected elsewhere, that do not fit the models could be viewed as atypical. In addition, comparisons between predicted and actual con-

TABLE 2 Comparison of Louisiana (LA) and Nationwide (NW) Data Bases. All elements and oxides in mg kg^{-1} except where noted.

	Cu		Zn		Pb		Cr		Ni		Co		As		Sb	
	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW
min.	2	4	4	23	3	9	9	20	10	4	3	6	0.5	1.5	0.2	0.1
max.	26	43	122	200	52	47	93	90	34	66	23	39	21.5	15.0	1.1	1.2
mean	18	20	82	88	33	23	65	51	22	25	13	17	6.6	7.0	0.9	0.6
median	20	17	94	85	33	22	75	50	24	23	14	17	5.3	6.0	0.9	0.6

	Se		Hg		Fe (wt. %)		Mn (wt. %)		Al (wt. %)		Ti (wt. %)		TOC (wt. %)[1]		LOI (wt. %)[2]	
	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW
min.	0.1	0.1	0.03	0.02	0.3	1.1	0.02	0.02	1.1	2.1	0.10	0.19	0.1	0.4	0.4	1.6
max.	0.7	0.9	0.17	0.13	4.3	6.1	0.16	0.10	9.0	8.1	0.60	0.66	3.3	5.5	10.9	13.5
mean	0.5	0.4	0.09	0.05	2.7	2.8	0.09	0.06	6.6	5.5	0.42	0.41	1.7	1.4	1.4	6.4
median	0.6	0.2	0.09	0.04	2.8	2.6	0.09	0.06	7.9	5.7	0.45	0.43	1.9	1.0	7.3	3.8

	OOM (wt. %)[3]		%<125µm		%<63µm		%<16µm		%<2µm		Mz (µm)[4]		S.A. (m^2 g^{-1})[5]	
	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW
min.	0.3	1.2	45.1	32.1	2.0	12.4	0.9	5.7	0.2	0.4	15.2	17.0	1.2	4.1
max.	7.7	8.0	96.4	99.3	92.5	97.1	64.7	54.7	19.1	24.7	107	125	48.7	29.5
mean	4.6	3.5	87.4	73.0	75.0	52.3	41.2	27.0	7.9	5.8	36.5	65.0	30.4	11.2
median	5.4	2.7	94.8	71.5	85.0	50.8	48.9	27.0	7.6	3.9	21.3	70.0	34.7	9.9

	$Mn.MnO_2$ [6]		$Fe.MnO_2$ [7]		$Fe.Fe_2O_3$ [8]		∑Ex.Fe [9]		∑Ex.Mn [10]	
	LA	NW	LA	NW	LA	NW	LA	NW	LA	NW
min.	20	5	60	110	300	790	550	1000	170	40
max.	280	350	1700	1300	3000	9000	9700	17 500	1300	900
mean	123	74	1100	480	4500	3600	6100	6100	680	400
median	115	40	1400	470	3200	2200	7100	4100	650	350

TOC (wt. %)[1] - total organic carbon
LOI (wt. %)[2] - loss on ignition
OOM (wt. %)[3] - other organic matter
Mz (µm)[4] - mean grain size
S.A. (m^2 g^{-1})[5] - surface area

$Mn{\cdot}MnO_2$ [6] - manganese oxides
$Fe{\cdot}MnO_2$ [7] - reactive iron
$Fe{\cdot}Fe_2O_3$ [8] - amorphous iron oxides
∑Ex.Fe [9] - total extractable iron
∑Ex.Mn [10] - total extractable manganese

centrations (the absolute value of individual residuals when converted from log to arithmetic space) also might help identify atypical samples, even if they marginally fit the models. For example, two samples from geothermal areas did not fit the models for several elements (e.g., As). The lack of fit could reflect 'natural' perturbations to background sediment-associated trace element concentrations. If samples were collected in areas where anthropogenic affects were suspected, they could be evaluated in the same way as the 'average' samples, that is by comparing the predicted concentrations with measured concentrations (significant differences between the two could indicate a potentially affected site). Since the models were developed from an environmentally diverse suite of sediment samples, they are probably applicable to many aquatic systems. A data set from a large area of diverse hydrology and geology, or a data set from a relatively small one, might require modification of the calculated model coefficients to better explain local chemical variances, but the independent variables identified in the original models would probably still be applicable. Regardless, in either their original or modified form, the models could be used as a screening/reconnaissance tool to initially identify sites or specific trace elements requiring further evaluation.

MODEL TESTING AND EVALUATION

The utility of sediment-trace element geochemical models for the determination of local trace element background levels was tested using data collected from a small drainage basin in Louisiana. The Mz's for all the Louisiana samples were <125µm; therefore, the <125µm models were used to attempt to calculate local background levels (Table 2). Initially, the calculated concentrations were about double the measured concentrations; thus, the nationwide model coefficients needed to be recalculated. These recalculations should be viewed as a calibration exercise intended to account for local conditions because although the median trace element concentrations for the Louisiana samples were similar to those for the nationwide samples used to calculate the models, their geochemical factors differed significantly (Table 2). The Louisiana samples are significantly finer-grained, have larger surface areas, more organic matter, and more reactive Fe, amorphous Fe oxides, and total extractable Fe than the nationwide samples. Seven of the calibrated Louisiana models were the same (included all the nationwide independent variables but had different coefficients) or simpler (included fewer of the nationwide independent variables with different coefficients), while three of the calibrated Louisiana models required alteration of the independent variables relative to the nationwide models (Table 3).

The agreement between the fitted and measured concentrations from the Louisiana study are quite good. Out of 120 data pairs (measured and model-calculated concentrations) only two (one for Hg, the other for As) did not fall within 10% of each other. The sites of these non-matching data pairs were identified as potentially affected. The elevated Hg level occurred at a site where rice seed had been traditionally treated with mercurial compounds for preservation purposes. This site is also downstream from an oil refinery where mercurial compounds have been employed as a bactericide. The elevated As level occurred at a site where some urban runoff occurs. Although the original models required recalibration to better account for local geochemical variances, recalibration should not detract from the view that sediment-trace element models could be used to establish local trace element baseline concentrations and to identify affected sites requiring further evaluation.

TABLE 3Nationwide Models Compared with the Louisiana Sample Models.

Element	Source	Model	R	R^2
Cu	NW[1]	Cu = .674Al + .367LOI + .205Fe·Fe_2O_3 - 1.87	.93	.84
	LA[2]	Cu = 1.88Al - .488LOI + .085	.99	.97
Zn	NW	Zn = .983Al + .263Fe·MnO_2 + .255LOI + .329	.94	.87
	LA	Zn = 1.867Al + .852Fe·MnO_2 - 1.106LOI - 1.348	.99	.98
Pb	NW	Pb = .351SA + .383OOM + .603Ti + .329	.86	.70
	LA	Pb = 1.384SA - .507OOM - .509Ti - .386	.99	.98
Cr	NW	Cr = .580OOM + .442Fe - .151SA + 1.347	.91	.80
	LA	Cr = .499OOM + .320Fe + 1.355	.99	.99
Ni	NW	Ni = .963Al + .248TOC + .648	.96	.91
	LA	Ni = 1.652Al - .297TOC + .003	.97	.92
Co	NW	Co = 1.661Ti + .089%<2µm + 1.76	.89	.77
	LA	Co = .933Fe·Fe_2O_3 - .257%<2µm - .197Mn·MnO_2 - 1.497	.97	.90
As	NW	As = 1.282Fe + %<125µm + .690	.88	.74
	LA	As = 2.19Fe - 3.466%<125µm + 6.589	.99	.96
Sb	NW	Sb = 1.013Al + .465%<63µm + .145Mn·MnO_2 - 2.062	.88	.73
	LA	Sb = .402%<63µm - .812	.95	.90
Se	NW	Se = .920OOM + .485SA + .616Ti - 1.255	.88	.74
	LA	Se = 1.196Fe·Fe_2O_3 -1.195SA+ 1.907Ti - 2002	.98	.94
Hg	NW	Hg = .605Fe·Fe_2O_3 + .091Mn·MnO_2 - 3.613	.89	.76
	LA	Hg = .420TOC + .254%<2µm - 1.408	.92	.81

[1] nationwide data base models for samples in which Mz is <125µm

[2] calibrated models for the Louisiana samples, all of which had Mz's <125µm

Model Key

Fe = total Fe
Al = total Al
Ti = total Ti
LOI = loss on ignition
TOC = total organic carbon

OOM = other organic matter
Fe·MnO_2 = reactive iron
Fe·Fe_2O_3 = Fe oxide
Mn·MnO_2 = Mn oxide
SA = surface area

ADDITIONAL MODEL CONFIGURATIONS AND USES

The original models were developed using bed sediment samples and their measured total (≥95% of the concentration present) trace element concentrations. It seems reasonable that a similar set of models could be developed using suspended sediments instead of bed sediments or for measured concentrations determined by some less rigorous analytical procedure, should this prove desirable. Further, similar models might also be constructed using some measure of bio- or environmental availability as the dependent variable, instead of a trace element concentration.

Models of the type developed and tested in this study also might be used to assess water-quality monitoring data. In this context, they could provide a means of evaluating outlying trace element concentrations in terms of either natural or anthropogenic environmental perturbations. For example, if a series of monthly bed or suspended sediment samples were collected and analyzed over a reasonable time period (e.g., 2 to 3 years) at a selected monitoring site, a range of expected trace element concentrations would result. At the same time, models of the type described in this study also could be developed. Data from ensuing monitoring activities could then be evaluated, if necessary, by using the models. Thus, if a monitoring sample contained a trace element concentration within the established range for the site, no further work would be required. On the other hand, if the measured concentration fell outside the analytical confidence limits of the established range, then the factors incorporated in the model would be determined and entered. If the model predicts the apparent outlying concentration, then it is likely that the system has not changed appreciably, and that the initial chemical range established for the site simply was not sufficiently broad to encompass the normal range of concentrations for the trace element of interest. However, if the model fails to predict the outlying concentration, the presence of some new factor(s) exerting a substantial influence on the sediment chemistry of the system might be indicated. This would warrant a re-examination of the factors contained in the model and how they relate to the site. It also might lead to a search for a new source(s) of the trace element in question.

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